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An accurate General Method to Correlate Saturated Vapor Pressure of Pure Substances

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In this study, a generalized equation is presented to calculate vapor pressure of pure substances as a function of reduced temperature, critical pressure, and acentric factor. With the presented model, vapor pressures have been calculated and evaluated with NIST data bank for 70 pure substances for about 14000 data points, and the overall average absolute percentage deviation has been only 0.783%. Also the accuracy of obtained model has been evaluated with mostly used equations and the results indicate the superiority of the proposed model against other methods used in this work.

Keywords: General equation, Vapor pressure, Pure substances, Thermodynamic properties

INTRODUCTION

Vapor-pressure equations try to provide the temperature dependence of the saturated pressure of a fluid along the (liquid + vapor) coexistence curve. Since the Clapeyron equation was proposed in 1834, there has been a plethora of vapor-pressure equations described for both correlating and predicting data of pure fluids [1].

Most oil and gas processing operations such as oil refinery requires the vapor pressure data for estimation of phase equilibrium. In combustion modeling, vapor pressure also plays an important role. The vapor pressure or equilibrium vapor pressure is a good indication of a liquid's evaporation rate. In numerical simulations, a change in fuel vapor pressure may result in significant changes in the fuel atomization and evaporation rates, and thereby the subsequent combustion and emission formation processes [2].

Due to the absence and the limited range of vapor pressure data in the literature, some researchers have used different vapor pressures correlations to estimate parameters in equations of state [1,3-8]. Numerous empirical vapor-

pressure equations have been published, the best known are those of Wagner [9], Clausius, Antoine, Frost-Kalkwarf, Cox, Gomez-Thodos, Lee-Kesler, Wagner, Ambrose-Walton, Riedel [10,11], Lemmon-Goodwin [12] Voutsas *et al.* [8], and Mejbri *et al.* [3]. The most common of all is Antoine type equation [13], which has three-parameters, but is valid only within a limited temperature range.

The Wagner equation is considered as a great contribution in vapor pressure equations research, because it can represent with high accuracy data for many substances over the entire liquid-vapor range from the triple point to the critical point. Wagner method has some constant parameters for each substance. This method and also Mejbri *et al.* [3] and Velasco *et al.* [1] methods are not present a general model with constant coefficients for all pure substances.

In this work we propose a general model with constant parameters for all pure substances based on liquid-vapor equilibrium data bank that accurately reproduces the vapor pressure behavior over a wide range of the liquid-vapor coexistence region. Based on this model a corresponding-state is established. The source of vapor pressure data used in this study is the NIST Chemistry WebBook [14].

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METHODOLOGY

Antoine Vapor Pressure Model

The Antoine vapor pressure model was modified based on the Clapeyron equation. It has been widely used to estimate the vapor pressure over limited temperature ranges [13]. The proposed model is shown below:

$$\ln P_{vp} = A - \frac{B}{T + C} \quad (1)$$

where, P_{vp} is the vapor pressure (mmHg), T is the temperature ($^{\circ}\text{C}$) and the constant values of A , B and C for some species are presented in Appendix A in [10].

Lee-Kesler's Method

The Lee-Kesler's method [10] is one of the successful methods to correlate the vapor pressure using the three-parameter formulations,

$$\ln P_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) \quad (2)$$

$$f^{(0)} = 5.92714 - \frac{6.09648}{T_r} - 1.28862 \ln T_r + 0.169347 T_r^6 \quad (3)$$

$$f^{(1)} = 15.2518 - \frac{15.6875}{T_r} - 13.4721 \ln T_r + 0.43577 T_r^6 \quad (4)$$

where P_{vpr} is the reduced vapor pressure which equals to P/P_c , and P_c is the critical pressure (pascal), ω is the acentric factor, and T_r is the reduced temperature which equals to T/T_c , where T_c is the critical temperature (K) of the fluid. Values for T_c and P_c can be found in the literature for many pure substances [11,15-17].

Ambrose-Walton Corresponding States Method

Ambrose and Walton [11] developed another representation of the Pitzer expansion with an additional term $f^{(2)}(T_r)$,

$$\ln P_{vpr} = f^{(0)}(T_r) + \omega f^{(1)}(T_r) + \omega^2 f^{(2)}(T_r) \quad (5)$$

$$f^{(0)} = \frac{-5.97616\tau + 1.29874\tau^{1.5} - 0.60394\tau^{2.5} - 1.06841\tau^5}{T_r} \quad (6)$$

$$f^{(1)} = \frac{-5.03365\tau + 1.11505\tau^{1.5} - 5.41217\tau^{2.5} - 7.46628\tau^5}{T_r} \quad (7)$$

$$f^{(2)} = \frac{-0.64771\tau + 2.41539\tau^{1.5} - 4.26979\tau^{2.5} + 3.25259\tau^5}{T_r} \quad (8)$$

$$\omega = -\frac{\ln(P_c/1.01325) + f^{(0)}(T_{br})}{f^{(1)}(T_{br})} \quad (9)$$

where ω is the acentric factor, P_c is the critical pressure (bars) of the fluid, and $\tau = 1 - T_r$.

Riedel Corresponding States Method

Riedel [18] proposed a vapor pressure equation of the form:

$$\ln P_{vpr} = A + \frac{B}{T_r} + C \ln T_r + DT_r^6 \quad (10)$$

The T_r^6 term allows description of the inflection point of the vapor pressure curve in the high-pressure region. Parameters A , B , C , and D are functions of T , T_c , T_b , and P_c .

PROPOSED CORRELATION FOR VAPOR PRESSURE

We tried to find a general equation to calculate vapor-pressure of pure substances. There is a twelve-constant non linear correlation which reproduces high accuracy vapor-liquid equilibrium data, even at low reduced temperatures. After multiple regression analysis, an empirical model was suggested as follow:

$$\ln P_{vpr} = f^{(0)} + \omega f^{(1)} + \omega^2 f^{(2)} \quad (12)$$

$$f^{(0)}(T_r) = a_1 + \frac{a_2}{T_r} + a_3 T_r + a_4 T_r^{0.8} \quad (13)$$

$$f^{(1)}(T_r) = a_5 + \frac{a_6}{T_r} + a_7 T_r + a_8 T_r^{0.8} \quad (14)$$

$$f^{(2)}(T_r) = a_9 + \frac{a_{10}}{T_r} + a_{11} T_r + a_{12} T_r^{0.8} \quad (15)$$

where P_{vpr} is reduced vapor pressure and equals to P/P_c , $T_r = T/T_c$ is the reduced temperature, and ω is acentric factor. a_1 to a_{12} (presented in Table 1) are tuned coefficients that have been determined using Marquardt-Levenberg algorithm minimizing the sum of the squared differences between the

Table 1. Tuned Coefficients of Proposed Model

Coeff.	Value	Standard deviation
a_1	14.7114	0.08880
a_2	-6.7632	0.01254
a_3	26.5948	0.26988
a_4	-34.5428	0.34567
a_5	49.1821	0.56822
a_6	-14.6979	0.08211
a_7	87.9972	0.69347
a_8	-122.4950	0.97704
a_9	6.6828	0.84754
a_{10}	-1.8259	0.21134
a_{11}	7.8256	0.42699
a_{12}	-12.7191	1.08420

values of the observed and correlated values of the dependent variables.

We carried out calculations for 70 pure substances. The criteria for comparisons are AARD%, ARD%, AAD and RMSD, calculated as follows:

$$AARD\% = \frac{1}{N} \sum_{i=1}^N \left| \frac{P_{i,\text{exp}} - P_{i,\text{calc}}}{P_{i,\text{exp}}} \right| \times 100 \quad (16)$$

$$ARD\% = \frac{1}{N} \sum_{i=1}^N \left(\frac{P_{i,\text{exp}} - P_{i,\text{calc}}}{P_{i,\text{exp}}} \right) \times 100 \quad (17)$$

$$AAD = \frac{1}{N} \sum_{i=1}^N |P_{i,\text{exp}} - P_{i,\text{calc}}| \quad (18)$$

$$RMSD = \frac{1}{N} \sqrt{\sum_{i=1}^N \left(\frac{P_{i,\text{exp}} - P_{i,\text{calc}}}{P_{i,\text{exp}}} \right)^2} \times 100 \quad (19)$$

RESULTS AND DISCUSSION

We carried out calculations for 70 pure substances. The values of the vapor pressure, temperature, critical pressure, critical temperature, boiling point, and acentric factor, were taken from data bank (NIST Chemistry WebBook, 2005) [14]. The number of data points, temperature ranges, critical temperature, critical pressure, and acentric factor for each substance is presented in Table 2.

To compare the accuracy of the presented empirical model, calculated vapor pressures for all substances versus corresponded values in data bank are presented in Fig. 1.

Table 2. Main Characteristics of the Considered Substances

Substance	Data points	T_{min}	T_{max}	T_c (K)	P_c (bar)	ω
N ₂	200	63.2	125.9	126.2	33.9	0.04
para Hydrogen	200	13.8	32.9	32.94	12.838	-0.218
Deuterium	200	18.7	38.34	38.34	16.653	-0.175
H ₂	200	13.9	33	33.15	12.964	-0.219
O ₂	200	54.4	154.1	154.58	50.43	0.022
Flourine	200	53.5	144.4	144.41	51.724	0.045
CO	200	68.2	132.9	132.86	34.935	0.05
CO ₂	200	216.6	304.1	304.13	73.773	0.224
N ₂ O	200	182.3	309.5	309.52	72.45	0.162
C ₁	200	90.7	190.6	190.56	45.992	0.011
C ₂	200	90.4	305.3	305.33	48.718	0.099
Ethene	200	104	282.4	282.35	50.418	0.087
C3	200	85.5	369.8	369.83	42.477	0.152
Propene	200	100	365.6	365.57	46.646	0.141

Table 2. Continued

Propyne	200	273	402.4	402.38	56.26	0.204
Cyc-Propane	200	273	398.3	398.3	55.797	0.131
n-C ₄	200	134.9	425.1	425.13	37.96	0.201
i-C ₄	200	113.7	407.8	407.81	36.29	0.184
n-C ₅	200	143.5	469.7	469.7	33.7	0.251
2-met-Butane	200	112.7	460.4	460.35	33.957	0.23
2,2-dimethyl-propane	200	256.6	433.7	433.74	31.96	0.196
n-C ₆	200	177.8	507.8	507.82	30.34	0.299
2-methyl pentane	200	121.5	497.7	497.7	30.4	0.28
cyc-Hexane	200	279.5	553.6	553.64	40.75	0.209
n-C ₇	200	182.6	540.1	540.13	27.36	0.349
n-C ₈	200	216.4	569.3	569.32	24.97	0.393
n-C ₉	200	219.7	594.6	594.55	22.81	0.443
n-C ₁₀	200	243.5	617.7	617.7	21.03	0.488
n-C ₁₂	200	263.6	658.1	658.1	18.17	0.574
He	200	2.2	5.2	5.2	2.275	-0.382
Ne	200	24.6	44.5	44.49	26.786	-0.039
Ar	200	83.8	150.7	150.69	48.63	-0.002
Kr	200	115.8	209.5	209.48	55.25	-0.001
Xe	200	161.4	289.7	289.73	58.42	0.004
NH ₃	200	195.5	405.4	405.4	113.33	0.256
NF ₃	200	85	234	234	44.607	0.126
R11 (Trichlorofluoromethane)	200	162.6	469.5	471.11	44.076	0.189
R12 (Dichlorodifluoromethane)	200	116.1	383.8	385.12	41.361	0.18
R13 (Chlorotrifluoromethane)	200	92	300.9	302	38.79	0.172
R14 (Tetrafluoromethane)	200	98.9	226.8	227.51	37.5	0.179
R21 (Dichlorofluoromethane)	200	200	450.2	451.48	51.812	0.179
R22 (Chlorodifluoromethane)	200	115.7	368	369.3	49.9	0.206
R23 (Trifluoromethane)	200	118	298.4	299.29	48.32	0.263
R41 (Monofluoromethane)	200	175	316.6	317.28	58.97	0.201
R113 (Trichlorotrifluoromethane)	200	236.9	485.9	487.21	33.922	0.253
R114 (1,2-Dichlorotetrafluoroethane)	200	273.1	418.1	418.83	32.57	0.252
R115 (Chloropentafluoroethane)	200	173.8	351.3	353.1	31.2	0.252
R116 (Hexafluoroethane)	200	173.1	292.4	293.03	30.48	0.257
R123 (2,2-Dichloro-1,1,1-trifluoroethane)	200	166	455.4	456.83	36.618	0.282
R124 (1-Chloro-1,2,2,2-tetrafluoroethane)	200	120	394.1	395.43	36.243	0.288
R125 (Pentafluoroethane)	200	172.5	338.3	339.17	36.177	0.305
R134a (1,1,1,2-Tetrafluoroethane)	200	169.8	373.2	374.21	40.593	0.327

Table 2. Continued

R141b (1,1-Dichloro-1-fluoroethane)	200	169.7	475.9	477.5	42.12	0.22
R142b (1-Chloro-1,1-difluoroethane)	200	142.7	408.9	410.26	40.55	0.232
R143a (1,1,1-trifluoroethane)	200	161.3	344.9	345.86	37.61	0.262
R152a (1,1-Difluoroethane)	200	154.5	385.2	386.41	45.168	0.275
R218 (Octafluoropropane)	200	125.4	343.9	345.02	26.4	0.317
R227ea (1,1,1,2,3,3,3- heptafluoropropane)	200	146.3	374.8	375.95	29.99	0.354
R236ea (1,1,1,2,3,3-Hexafluoropropane)	200	242	411.6	412.44	35.02	0.379
R236fa (1,1,1,3,3,3-Hexafluoropropane)	200	179.5	396.9	398.07	32	0.377
R245ca (1,1,2,2,3-Pentafluoropropane)	200	200	443.9	447.57	39.25	0.354
R245fa (Pentafluoropropane)	200	200	426.1	427.2	36.4	0.372
RC318 (Octafluorocyclobutane)	200	233.3	387.6	388.38	27.775	0.355
Benzene	200	278.7	562.1	562.05	48.94	0.209
Toluene	200	178	591.7	591.75	41.263	0.266
C ₄ F ₁₀	200	189	386.3	386.33	23.234	0.374
SO ₂	200	197.7	430.6	430.64	78.84	0.256
H ₂ S	200	187.7	373.1	373.1	90	0.1
SF ₆	200	222.4	318.7	318.73	37.546	0.21
COS	200	134.3	378.8	378.77	63.7	0.098

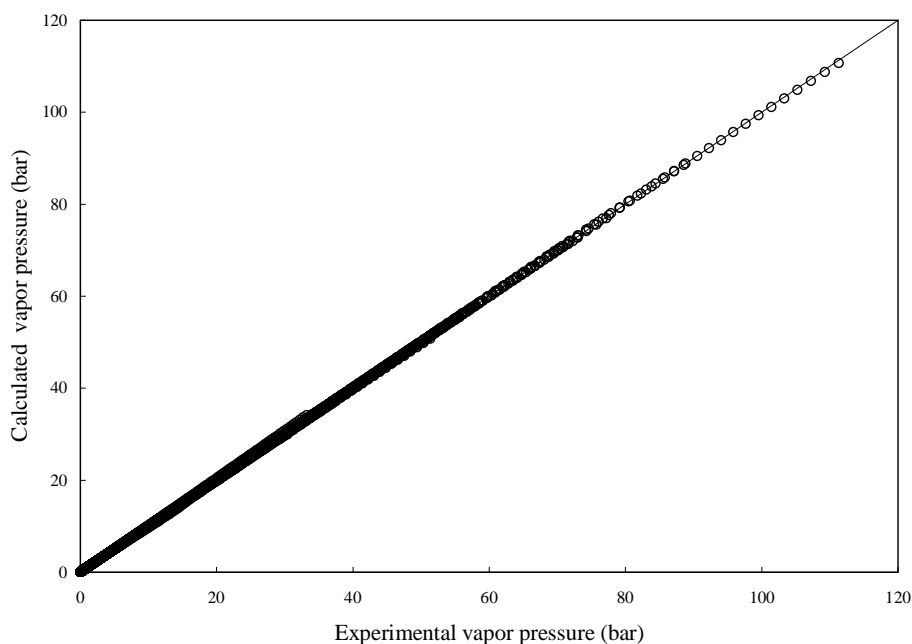


Fig. 1. Accuracy of presented model versus sources data.

In Table 3, the AARD% of vapor pressure calculated from the proposed and other models for each substance with respect to the values given by data bank is presented. This comparison shows that the presented model is more accurate than other methods for approximately all types of

pure substances considered in this study.

Where "N.A." means that the parameters of model are not available for the considered substances. Also in Table 4, the AAD% of vapor pressure calculated from the proposed and other models for each substance with respect to the

Table 3. Average Absolute Relative Deviation of the Values Obtained by Presented Model in Comparison with other Methods

Substance	Lee-Kesler	Ambrose-Walton	Riedel	Antoine	This study
N ₂	1.0985	0.5987	N. A.	4.4752	0.6276
para Hydrogen	0.2945	0.7958	1.2480	N. A.	1.2864
Deuterium	2.4502	2.2581	1.6157	14.4675	1.9108
H ₂	0.0595	0.5036	1.0895	1.6104	1.8768
O ₂	0.6862	1.2935	0.6578	1.4456	0.2631
Flourine	1.7073	3.3784	1.0076	1.5196	1.7719
CO	0.1950	0.7382	0.1299	2.6884	0.5428
CO ₂	0.2162	0.4888	14.5390	6.0116	0.4470
N ₂ O	0.1383	0.3440	0.1153	1.9845	0.2943
C ₁	0.7411	0.0338	0.7037	1.8611	0.3778
C ₂	1.8018	0.1635	1.3863	1.7730	1.6071
Ethene	0.8302	2.1224	1.0020	2.2928	1.1335
C ₃	3.7010	0.6509	4.9134	1.5900	0.7437
Propene	2.4042	2.4299	3.2827	0.2051	0.6475
Propyne	0.9124	0.6483	2.5109	8.4023	0.7114
Cyc-Propane	0.1301	0.0962	0.9214	1.4773	0.0977
n-C ₄	2.7186	0.8768	1.5028	0.5027	1.8040
i-C ₄	2.3180	1.5487	3.2082	1.0991	0.1989
n-C ₅	2.4801	0.7676	1.9307	1.2560	1.5775
2-met-Butane	4.3997	0.9898	5.7135	0.1652	1.5547
2,2-Dimethyl-propane	0.1892	0.2906	0.1367	0.1179	0.2404
n-C ₆	2.6130	0.7093	1.1094	0.1743	1.3386
2-Methyl pentane	4.4317	0.7728	6.5254	0.1506	1.4839
cyc-Hexane	0.2048	0.9342	0.2394	0.0569	0.7580
n-C ₇	1.8279	0.3379	1.8896	0.1827	0.4029
n-C ₈	1.0722	1.5144	1.3463	0.6927	0.8683
n-C ₉	1.6138	0.5108	1.7806	2.4228	0.4024
n-C ₁₀	1.3800	0.4218	1.3354	0.1380	0.4621
n-C ₁₂	1.3888	1.2513	2.9645	0.0883	0.5670
He	6.1867	3.6751	4.6875	1.4196	1.4925
Ne	0.4010	0.1933	0.6227	2.0648	0.3408

Table 3. Continued

Ar	0.1548	0.2466	0.2737	0.4251	0.1777
Kr	0.1929	0.1235	0.4607	0.7106	0.1405
Xe	0.1419	0.1994	0.3470	0.2803	0.1823
NH3	2.6007	1.3339	1.6513	0.6900	1.5689
NF3	1.4398	0.5679	0.6954	0.4021	0.5078
R11	1.2231	1.4616	1.3930	0.4426	0.5837
R12	2.1819	1.6417	2.7547	4.0453	0.4969
R13	2.3240	2.9968	3.0997	11.7266	0.9945
R14	1.6171	0.1228	0.9141	1.4640	0.4460
R21	0.1763	1.5074	0.2642	2.1656	1.1722
R22	1.8346	1.0311	2.2490	0.2642	0.2361
R23	3.6254	1.7281	1.9250	1.5356	1.2388
R41	1.5569	0.8677	1.4442	1.2565	0.9649
R113	0.6816	0.6295	0.2786	1.0235	0.4184
R114	0.2436	0.1006	0.2662	0.2410	0.0759
R115	1.4222	0.3676	0.9251	0.5177	0.3208
R116	0.5412	0.0575	0.4034	1.1843	0.1114
R123	1.2774	1.8667	1.7947	N. A.	1.2440
R124	2.3099	1.9531	3.6906	0.9479	0.7943
R125	0.8073	0.3690	0.3464	4.2140	0.1955
R134a	1.7158	0.1263	0.7483	11.0496	0.4553
R141b	1.7258	3.1924	2.4801	N. A.	1.3897
R142b	1.4135	1.1321	1.4703	3.5243	0.4423
R143a	2.4183	0.9833	1.5651	1.8699	1.0038
R152a	3.8526	1.9859	2.1925	6.3103	1.5366
R218	1.3864	0.7849	1.1504	15.9391	0.2183
R227ea	1.2780	1.3868	1.5549	N. A.	0.8894
R236ea	1.8508	1.1632	1.5708	13.8099	1.2286
R236fa	0.5752	1.1707	0.6424	4.5100	0.8238
R245ca	1.8296	0.2534	0.6558	4.8948	0.6497
R245fa	0.2850	1.6200	0.7690	23.5820	1.2874
RC318	0.1347	0.5090	0.1431	1.2206	0.4675
Benzene	0.2255	1.0875	0.3124	1.3452	0.9107
Toluene	2.8685	0.5607	3.3767	4.8560	1.0810
C4F10	0.6019	1.3317	0.7974	2.2389	1.1088
SO2	1.0681	0.4905	0.3843	0.7494	0.2066
H2S	0.3591	0.5068	0.3521	2.5243	0.3977
SF6	0.5268	0.2387	1.2823	12.8639	0.3053
COS	1.0581	1.9778	1.3192	0.3660	0.9383

Table 4. Average Absolute Deviation (AAD) of the Values Obtained by Presented Model in Comparison with other Methods

Substance	Lee-Kesler	Ambrose-Walton	Riedel	Antoine	This study
2,2-Dimeth-prop	0.0074	0.0145	0.0079	0.5247	0.0103
2-Met pent	0.0159	0.0032	0.0152	0.1789	0.0054
2-Met-But	0.0415	0.0276	0.0450	0.1662	0.0058
Ar	0.0164	0.0197	0.0223	0.8079	0.0183
Benzene	0.0132	0.0154	0.0097	0.4179	0.0135
C1	0.0113	0.0019	0.0496	0.2822	0.0102
C10	0.0200	0.0031	0.0104	0.0835	0.0046
C12	0.0127	0.0039	0.0058	0.0731	0.0028
C2	0.0112	0.0031	0.0326	0.2133	0.0065
C3	0.0124	0.0012	0.0211	0.1810	0.0058
C4F10	0.0143	0.0317	0.0147	0.0571	0.0220
C7	0.0158	0.0029	0.0098	0.1477	0.0042
C8	0.0135	0.0050	0.0030	0.1476	0.0024
C9	0.0240	0.0075	0.0154	0.1006	0.0091
CO	0.0209	0.0297	0.0139	0.1357	0.0164
CO2	0.0659	0.1306	2.5813	0.3752	0.0225
COS	0.0252	0.0135	0.0473	0.4193	0.0078
cyc-hex	0.0080	0.0234	0.0091	0.3002	0.0163
Cyc-Prop	0.0269	0.0182	0.1098	0.8258	0.0194
Dutrium	0.1270	0.1190	0.1201	0.9157	0.0148
Ethene	0.0086	0.0153	0.0144	0.5145	0.0114
Flourine	0.1009	0.1123	0.0980	0.2970	0.0131
H2	0.0020	0.0078	0.0152	0.1314	0.0172
H2S	0.0280	0.0176	0.0642	1.3244	0.0164
He	0.0104	0.0053	0.0084	0.0102	0.0050
i-C4	0.0066	0.0081	0.0108	0.1328	0.0032
Kr	0.0090	0.0048	0.0537	1.2872	0.0199
N2	0.0442	0.0467	0.0832	0.6847	0.0326
N2O	0.0172	0.0388	0.0187	0.8837	0.0285
n-C4	0.0266	0.0107	0.0346	0.1478	0.0162
n-C5	0.0240	0.0083	0.0246	0.1305	0.0116
n-C6	0.0161	0.0052	0.0141	0.1944	0.0038
Ne	0.0105	0.0092	0.0334	0.9352	0.0200
NF3	0.0157	0.0224	0.0163	0.4195	0.0138
NH3	0.1018	0.0403	0.2093	1.8822	0.0480

Table 4. Continued

O2	0.0099	0.0103	0.0261	0.4313	0.0053
para h2	0.0033	0.0102	0.0184	N.A.	0.0188
Propene	0.0070	0.0088	0.0160	0.3051	0.0049
Propyne	0.1238	0.0861	0.2975	2.3200	0.0388
R11	0.0094	0.0114	0.0142	0.2941	0.0072
R113	0.0123	0.0094	0.0104	0.1075	0.0087
R114	0.0151	0.0131	0.0156	0.1792	0.0074
R115	0.0339	0.0388	0.0351	0.2079	0.0101
R116	0.0252	0.0040	0.0253	0.3027	0.0084
R12	0.0195	0.0044	0.0270	0.4842	0.0101
R123	0.0144	0.0060	0.0117	N.A	0.0044
R124	0.0093	0.0091	0.0067	0.0861	0.0062
R125	0.0115	0.0153	0.0093	0.5190	0.0098
R13	0.0141	0.0054	0.0182	1.0614	0.0091
R134a	0.0240	0.0049	0.0210	1.0627	0.0051
R14	0.0214	0.0177	0.0271	0.1941	0.0045
R141b	0.0100	0.0134	0.0102	N.A.	0.0123
R142b	0.0254	0.0072	0.0277	0.2142	0.0119
R143a	0.0415	0.0180	0.0486	0.3760	0.0229
R152a	0.0456	0.0197	0.0561	0.4900	0.0237
R21	0.0091	0.0192	0.0072	0.3274	0.0181
R218	0.0201	0.0060	0.0152	0.1056	0.0089
R22	0.0106	0.0122	0.0164	0.8151	0.0063
R227ea	0.0200	0.0018	0.0136	N.A.	0.0047
R23	0.0446	0.0179	0.0573	0.2240	0.0230
R236ea	0.2194	0.1845	0.2133	2.0899	0.0251
R236fa	0.0193	0.0050	0.0102	0.3540	0.0056
R245ca	0.0282	0.0042	0.0267	0.4663	0.0062
R245fa	0.0067	0.0265	0.0135	3.9746	0.0218
R41	0.1104	0.0738	0.1708	0.4720	0.0220
RC318	0.0062	0.0264	0.0126	0.1309	0.0247
SF6	0.0557	0.0242	0.1133	15.4258	0.0359
SO2	0.0392	0.0183	0.0485	0.3237	0.0117
Toluene	0.0406	0.0208	0.0460	0.2374	0.0131
Xe	0.0116	0.0118	0.0421	1.1947	0.0125

values given by data bank is presented to show how the model works for all considered pure substances. Compared values show that the presented model is more accurate than other methods for approximately all types of pure substances considered in this study.

Table 5 presents the statistical parameters including average absolute percentage relative deviation percentage (AARD%), average relative deviation, (ARD%), average absolute deviation (AAD), and root mean square deviation (RMSD) of the considered models and the proposed equation.

Figure 2 shows the cumulative frequency of the proposed model and different corresponding methods against average absolute relative deviations. Figure 2 also shows the accuracy of all considered methods in prediction of vapor pressure for more than 70 substances.

In probability theory and statistics, the cumulative distribution function (CDF), or just distribution function, describes the probability that a real-valued random variable AARD (in this case) with a given probability distribution will be found to have a value less than or equal to AARD. In the case of a continuous distribution, it gives the area

Table 5. Statistical Parameters of this Study Compared with other Methods

	AARD%	ARD%	AAD	RMSD
Antoine	3.144	-1.124	0.759	8.427
Ambros-Walton	1.011	0.898	0.023	2.360
Riedel	1.702	0.672	0.077	5.018
Lee-Kesler	1.453	0.291	0.029	3.373
This study	0.783	-0.026	0.014	1.388

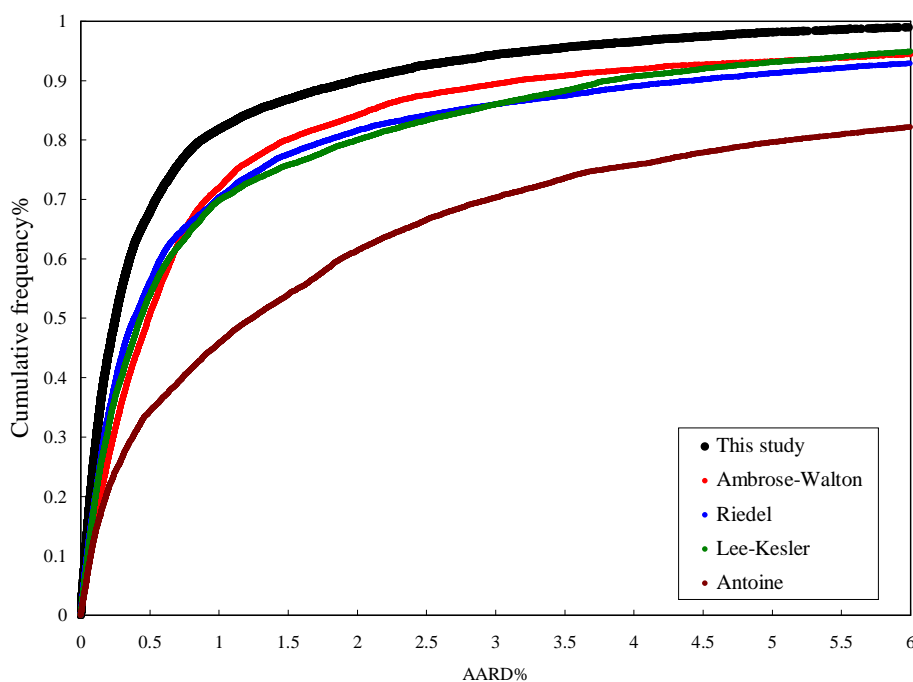


Fig. 2. AARD% of various methods in calculating vapor pressure as function of cumulative frequency.

under the probability density function from minus infinity to AARD. As shown in Fig. 2, the proposed equation is more accurate than other commonly used models in vapor pressure prediction.

The proposed method has successfully correlated 68% of all 14000 data with AARD % less than 0.5, and 90% of the data with AARD% less than 2. Only 1.8% of the vapor pressure data were correlated with AARD% of more than 5 by the presented method. Ambrose-Walton equation, that is the second accurate method, correlated 50% of the data with AARD% less than 0.5, and 84% of the data with AARD (%) less than 2. Hence, the superiority of this proposed method over the other corresponding states has been verified for all data available in data bank.

CONCLUSIONS

In order to simplicity and low deviations toward literature correlations for calculation the vapor pressure of the pure compounds, from the data of the reduced temperature, critical pressure, and acentric factor, a non linear correlation was recommended to estimate the vapor pressure of the pure substances more accurate than other commonly used models. Also various vapor pressure correlation methods were compared and evaluated. To validate the proposed method, the vapor pressures of 70 pure substances with 14000 data points were also examined and an overall average absolute percentage deviation of 0.783% was achieved.

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